Steven A. Corcelli

Professor, Department of Chemistry and Biochemistry
Associate Dean for Interdisciplinary Programs and Faculty Development, College of Science
University of Notre Dame
Notre Dame, IN 46556
Phone: (574) 631-2631
Email: scorcell@nd.edu
http://chemistry.nd.edu/people/steven-corcelli/

Education and Training

2002 – 2005	Postdoctoral Research Associate, Department of Chemistry, University of Wisconsin, Madison, Advisor: James L. Skinner
2002	Ph.D. in Chemistry, Yale University, Advisor: John C. Tully
1997	Sc.B. in Chemistry, Brown University, Advisor: Jimmie D. Doll

Academic Positions

2017 – present	Professor, Department of Chemistry and Biochemistry, University of Notre Dame
2011 – 2017	Associate Professor, Department of Chemistry and Biochemistry, University of Notre Dame
2005 – 2011	Assistant Professor, Department of Chemistry and Biochemistry, University of Notre Dame

Administrative Appointments

2019 – present	Associate Dean for Interdisciplinary Programs and Faculty Development, College of Science, University of Notre Dame
2019 – 2021	Fellow, Office of the Provost, University of Notre Dame
2016 – 2019	Associate Department Chair, Department of Chemistry and Biochemistry, University of Notre Dame
2012 – 2016	Director of Graduate Studies, Department of Chemistry and Biochemistry, University of Notre Dame

Awards and Honors

2021	Faculty Fellow, Kaneb Center for Teaching and Learning, University of Notre Dame
2020	Thomas P. Madden Award for Excellence in Teaching First-Year Undergraduates, University of Notre Dame
2019	Rev. Edmund P. Joyce, C.S.C. Award for Excellence in Undergraduate Teaching, University of Notre Dame
2019	Student Hosted Colloquium in Physical Chemistry, University of California, Berkeley
2018	Frontiers in Chemical Physics Lectures, The Ohio State University
2016	Fellow, American Chemical Society
2015	Director of Graduate Studies Award, University of Notre Dame

2012	Rev. Edmund P. Joyce, C.S.C. Award for Excellence in Undergraduate Teaching, University of Notre Dame
2011	Kavli Fellow, National Academy of Sciences and Alexander von Humboldt Foundation
2009	Sloan Research Fellowship
2009	National Science Foundation CAREER Award
2005	Camille and Henry Dreyfus New Faculty Award
2003	Ruth L. Kirschstein National Research Service Award
2002	Richard Wolfgang Prize (yearly award for the best Ph.D. thesis), Department of Chemistry, Yale University
1997	National Science Foundation Graduate Research Fellowship
1997	Sc.B., Magna Cum Laude with Honors, Brown University

Peer-Reviewed Journal Articles (85 total)

1. M. D. Hanson, J. A. Readnour, A. A. Hassanali, S. A. Corcelli, "Coupled Local Mode Approach for the Calculation of Vibrational Spectra: Application to Protonated Water Clusters," *Journal of Physical Chemistry Letters* **12**, 9226 (2021).

2. C. I. Drexler, O. M. Cracchiolo, R. L. Myers, H. I. Okur, A. L. Serrano, S. A. Corcelli, and P. S. Cremer, "Local Electric Fields in Aqueous Electrolytes," (Dor Ben-Amotz Festschrift) *Journal of Physical Chemistry B* **125**, 8484 (2021).

3. S. R. Hodge, S. A. Corcelli, and M. A. Berg, "Nonlinear Kinetics and Generalized Dynamical Modes: II. Application to a Simulation of Solvation Dynamics in an Ionic Liquid," *Journal of Chemical Physics* **155**, 024123 (2021).

4. D. Mendes de Oliveira, A. J. Brendt, T. C. Miller, S. A. Corcelli, and D. Ben-Amotz, "Spectroscopic and Structural Characterization of Water-Shared Ion-Pairs in Aqueous Sodium and Lithium Hydroxide," (Lawrence R. Pratt Festschrift) *Journal of Physical Chemistry B* **125**, 1439 (2021).

5. X.-X. Zhang, S. L. Brantley, S. A. Corcelli, and A. Tokmakoff, "DNA Minor-Groove Binder Hoechst 33258 Destabilizes Base-Pairing Adjacent to its Binding Site," *Communications Biology* **3**, 525 (2020).

6. O. M. Cracchiolo, D. K. Geremia, S. A. Corcelli, and A. L. Serrano, "Hydrogen Bond Exchange and Ca^{2+} Binding of Aqueous *N*-Methylacetamide Revealed by 2DIR Spectroscopy," *Journal of Physical Chemistry B* **124**, 6947 (2020).

7. A. M. Silsky-Devlin, J. P. Petersen, J. Liu, S. A. Corcelli, S. A. Kandel, "Methylisatin Structural Isomers Have Different Kinetic Pathways to Self-Assembly," *Journal of Physical Chemistry C* **124**, 17717 (2020).

8. C. R. Baiz, B. Błasiak, J. Bredenbeck, M. Cho, J.-H. Choi, S. A. Corcelli, A. G. Dijkstra, C.-J. Feng, S. Garrett-Roe, N.-H. Ge, M. W. D. Hanson-Heine, J. D. Hirst, T. L. C. Jansen, K. Kwac, K. J. Kubarych, C. H. Londergan, H. Maekawa, M. Reppert, S. Saito, S. Roy, J. L. Skinner, G. Stock, J. E. Straub, M. C. Thielges, K. Tominaga, A. Tokmakoff, H. Torii, L. Wang, L. J. Webb, and M. T. Zanni, "Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction," (featured on the cover) *Chemical Reviews* **120**, 7152 (2020).

9. D. J. Floisand, T. C. Miller, and S. A. Corcelli, "Dynamics and Vibrational Spectroscopy of Alcohols in Ionic Liquids: Methanol and Ethanol," *Journal of Physical Chemistry B* **123**, 8113 (2019).

10. A. A. Kananenka, K. Yao, S. A. Corcelli, and J. L. Skinner, "Machine Learning for Vibrational Spectroscopic Maps" *Journal of Chemical Theory and Computation* **15**, 6850 (2019).

11. C. A. Daly Jr., C. Allison, and S. A. Corcelli, "Modeling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: IV. Temperature Dependence," (Pacific Conference on Spectroscopy and Dynamics Virtual Special Issue) *Journal of Physical Chemistry B* **123**, 3797 (2019).

12. J. P. Petersen, R. D. Brown, A. M. Silski, S. A. Corcelli, and S. A. Kandel, "Complex Structures Resulting from Carboxylic Acid Self-Assembly: Comparison of 2-Naphthoic Acid to Quinaldic Acid and 3-Quinoline Carboxylic Acid," *Journal of Physical Chemistry C* **123**, 13610 (2019).

13. C. M. Ayres, E. T. Abualrous, A. Bailey, C. Abraham, L. M. Hellman, S. A. Corcelli, F. Noé, T. Elliott, and B. M. Baker, "Dynamically Driven Allostery in MHC Proteins: Peptide-Dependent Tuning of Class I MHC Global Flexibility," *Frontiers in Immunology* **10**, 966 (2019).

14. C. I. Drexler, T. C. Miller, B. A. Rogers, Y. C. Li, C. A. Daly Jr., T. Yang, S. A. Corcelli, and P. S. Cremer, "Counter Cations Affect Transport in Aqueous Hydroxide Solutions with Ion Specificity," *Journal of the American Chemical Society* **141**, 6930 (2019).

15. A. M. Silski, J. P. Petersen, R. D. Brown, S. A. Corcelli, and S. A. Kandel, "STM Investigation of 2D Polymorphism of Structural Isomers," *Journal of Physical Chemistry C* **122**, 25467 (2018).

16. R. G. Mullen, S. A. Corcelli, and E. J. Maginn, "Reaction Ensemble Monte Carlo Simulations of CO_2 Absorption in the Reactive Ionic Liquid Triethyl(octyl)phosphonium 2-Cyanopyrrolide," *Journal of Physical Chemistry Letters* **9**, 5213 (2018).

17. T. Brinzer, C. A. Daly Jr., C. Allison, S. Garrett-Roe, and S. A. Corcelli, "Modelling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: III. Dynamics and Spectroscopy," *Journal of Physical Chemistry B* **122**, 8931 (2018).

18. Z. L. Terranova and S. A. Corcelli, "Decompositions of Solvent Response Functions in Ionic Liquids: A Direct Comparison of Equilibrium and Nonequilibrium Methodologies," *Journal of Physical Chemistry B* **122**, 6823 (2018).

19. C. A. Daly Jr., T. Brinzer, C. Allison, S. Garrett-Roe, and S. A. Corcelli, "Enthalpic Driving Force for the Selective Absorption of CO_2 by an Ionic Liquid," *Journal of Physical Chemistry Letters* **9**, 1393 (2018).

20. R. D. Brown, S. A. Corcelli, and S. Alex Kandel, "Structural Polymorphism as the Result of Kinetically Controlled Self-Assembly," *Accounts of Chemical Research* **51**, 465 (2018).

21. T. Zhang, S. L. Brantley, D. Verreault, R. Dhankani, Steven A. Corcelli, and Heather C. Allen, "pH and Salt Effects on the Speciation and Surface-pK_a of Phosphatidic Acid Monolayers at the Air-Aqueous Interface," *Langmuir* **34**, 530 (2018).

22. C. A. Daly Jr., L. M. Streacker, Y. Sun, S. R. Pattenaude, A. Hassanali, P. B. Petersen, S. A. Corcelli, and D. Ben-Amotz, "Decomposition of the Experimental Raman and Infrared Spectra of Acidic Water into Proton, Special Pair, and Counterion Contributions," *Journal of Physical Chemistry Letters* **8**, 5246 (2017).

23. R. D. Brown, R. C. Quardokus, N. A. Wasio, J. P. Petersen, A. M. Silski, S. A. Corcelli, and S. A. Kandel, "Non-intuitive Clustering of 9,10-Phenanthrenequinone on Au(111)," *Beilstein Journal of Nanotechnology* **8**, 1801 (2017).

24. A. M. Silski, R. D. Brown, J. P. Petersen, J. M. Coman, D. A. Turner, S. A. Corcelli, and S. Alex Kandel, "CH ⋯ O Hydrogen Bonding in Pentamers of Isatin" *Journal of Physical Chemistry C* **121**, 21520 (2017).

25. C. M. Ayres, S. A. Corcelli, and B. M. Baker, "Peptide and Peptide-Dependent Motions in MHC Proteins: Biophysical Underpinnings and Immunological Implications," *Frontiers in Immunology* **8**, 935 (2017).

26. R. D. Brown, J. M. Coman, J. A. Christie, R. P. Forrest, C. S. Lent, S. A. Corcelli, K. W. Henderson, and S. A. Kandel, "Evolution of Metastable Clusters into Ordered Structures for 1-1′-Ferrocenedicarboxylic Acid on the Au(111) Surface," *Journal of Physical Chemistry C* **121**, 6191 (2017).

27. C. M. Ayres, T. P. Riley, S. A. Corcelli, and B. M. Baker, "Modeling Peptide Fluctuations in Immunologic Recognition," *Journal of Chemical Information and Modeling* **57**, 1990 (2017).

28. M. L. McDermott, H. Vanselous, S. A. Corcelli, and P. B. Petersen, "DNA's Chiral Spine of Hydration," *ACS Central Science* **3**, 708 (2017).

29. E. J. Berquist, C. A. Daly Jr., T. Brinzer, K. K. Bullard, Z. M. Campbell, S. A. Corcelli, S. Garrett-Roe, and D. S. Lambrecht, "Modelling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: I. *Ab Initio* Calculations," *Journal of Physical Chemistry B* **121**, 208 (2017).

30. C. A. Daly Jr., E. J. Berquist, T. Brinzer, S. Garrett-Roe, D. S. Lambrecht, and S. A. Corcelli, "Modelling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: II. Spectroscopic Map," *Journal of Physical Chemistry B* **120**, 12633 (2016).

31. M. C. Sherman and S. A. Corcelli, "Nonadiabatic Transition Path Sampling," *Journal of Chemical Physics* **145**, 034110 (2016).

32. E. P. Blair, S. A. Corcelli, and C. S. Lent, "Electric-Field-Driven Electron-Transfer in Mixed-Valence Molecules," *Journal of Chemical Physics* **145**, 014307 (2016).

33. C. M. Ayres, D. R. Scott, S. A. Corcelli, and B. M. Baker, "Differential Utilization of Binding Loop Flexibility in T Cell Receptor Ligand Selection and Cross-Reactivity," *Scientific Reports* **6**, 25070 (2016).

34. S. D. Verma, S. A. Corcelli, and M. A. Berg, "Rate and Amplitude Heterogeneity in the Solvation Response of an Ionic Liquid," *Journal of Physical Chemistry Letters* **7**, 504 (2016).

35. J. A. Christie, R. P. Forrest, S. A. Corcelli, N. A. Wasio, R. C. Quardokus, R. D. Brown, S. A. Kandel, Y. Lu, C. S. Lent, K. W. Henderson, "Synthesis of a Neutral Mixed-Valence Diferrocenyl Carborane for Molecular

Quantum-Dot Cellular Automata Applications," (communication) *Angewandte Chemie International Edition* **54**, 15448 (2015).

36. D. J. Floisand and S. A. Corcelli, "Computational Study of Phosphate Vibrations as Reporters of DNA Hydration" *Journal of Physical Chemistry Letters* **6**, 4012 (2015).

37. N. A. Wasio, R. C. Quardokus, R. D. Brown, R. P. Forrest, C. S. Lent, S. A. Corcelli, J. A. Christie, K. W. Henderson, and S. A. Kandel, "Cyclic Hydrogen Bonding in Indole Carboxylic Acid Clusters," *Journal of Physical Chemistry C* **119**, 21011 (2015).

38. R. C. Quardokus, N. A. Wasio, R. D. Brown, J. A. Christie, K. W. Henderson, R. P. Forrest, C. S. Lent, S. A. Corcelli, and S. A. Kandel, "Hydrogen-Bonded Clusters of 1,1'-Ferrocenedicarboxylic Acid on Au(111) Are Initially Formed in Solution," *Journal of Chemical Physics* **142**, 101927 (2015).

39. M. C. Sherman and S. A. Corcelli, "Thermal Equilibrium Properties of Surface Hopping with an Implicit Langevin Bath," *Journal of Chemical Physics* **142**, 024110 (2015).

40. D. A. Hines, R. P. Forrest, S. A. Corcelli, and P. V. Kamat, "Predicting the Rate Constant of Electron Tunneling Reactions at the CdSe-TiO_2 Interface," (John R. Miller and Marshall D. Newton Festschrift) *Journal of Physical Chemistry B* **119**, 7439 (2015).

41. R. Adhikary, J. Zimmermann, J. Liu, R. P. Forrest, T. D. Janicki, P. E. Dawson, S. A. Corcelli, and F. E. Romesberg, "Evidence of an Unusual N-H---N Hydrogen Bond in Proteins" (communication) *Journal of the American Chemical Society* **136**, 13474 (2014).

42. F. Duan, J. Duitama, S. Al Seesi, C. M. Ayres, S. A. Corcelli, A. P. Pawashe, T. Blanchard, D. McMahon, J. Sidney, A. Sette, B. M. Baker, I. I. Mandoiu, and P. K. Srivastava, "Genomic and Bio-Informatic Profiling of Mutational Neo-Epitopes Reveals New Rules to Predict Anti-Cancer Immunogenicity," *Journal of Experimental Medicine* **211**, 2231 (2014).

43. R. C. Quardokus, N. A. Wasio, J. A Christie, K. W. Henderson, R. P. Forrest, C. S. Lent, S. A. Corcelli, and S. A. Kandel, "Hydrogen-Bonded Clusters of Ferrocenecarboxylic Acid on Au (111)" (communication) *Chemical Communications* **50**, 10229 (2014).

44. S. A. Corcelli, B. B. Laird, J. G. Saven, and J. R. Schmidt, "Tribute to James L. Skinner," (James L. Skinner Festschrift) *Journal of Physical Chemistry B* **118**, 7669 (2014).

45. Z. L. Terranova and S. A. Corcelli, "A Molecular Dynamics Investigation of the Vibrational Spectroscopy of Isolated Water in an Ionic Liquid," (James L. Skinner Festschrift) *Journal of Physical Chemistry B* **118**, 8264 (2014).

46. N. A. Wasio, R. C. Quardokus, R. P. Forrest, C. S. Lent, S. A. Corcelli, J. A. Christie, K. W. Henderson, and S. A. Kandel, "Self-Assembly of Hydrogen-Bonded Two-Dimensional Quasicrystals," *Nature* **507**, 86 (2014).

47. Z. L. Terranova and S. A. Corcelli, "On the Mechanism of Solvation Dynamics in Imidazolium-Based Ionic Liquids," (Michael D. Fayer Festschrift) *Journal of Physical Chemistry B* **117**, 15659 (2013).

48. R. C. Quardokus, N. A. Wasio, R. P. Forrest, C. S. Lent, S. A. Corcelli, J. A. Christie, K. W. Henderson, and S. A. Kandel, "Adsorption of Diferrocenylacetylene on Au(111) Studied by Scanning Tunneling Microscopy," *Physical Chemistry Chemical Physics* **15**, 6973 (2013).

49. D. R. Scott, C. F. Vardeman II, S. A. Corcelli, and B. M. Baker, "Limitations of Time-Resolved Fluorescence Suggested by Molecular Simulations: Assessing the Dynamics of T Cell Receptor Binding Loops," *Biophysical Journal* **103**, 2532 (2012).

50. N. A. Wasio, R. C. Quardokus, R. P. Forrest, S. A. Corcelli, Y. Lu, C. S. Lent, F. Justaud, C. Lapinte, S. A. Kandel, "STM Imaging of Three-Metal-Center Molecules: Comparison of Experiment and Theory for Two Mixed-Valence Oxidation States," *Journal of Physical Chemistry C* **116**, 25486 (2012).

51. Z. L. Terranova and S. A. Corcelli, "Monitoring Intramolecular Proton Transfer with Two-Dimensional Infrared Spectroscopy," *Journal Physical Chemistry Letters* **3**, 1842 (2012).

52. D. R. Scott, O. Y. Borbulevych, K. H. Piepenbrink, S. A. Corcelli, and B. M. Baker, "Disparate Degrees of Hypervariable Loop Flexibility Control T-Cell Receptor Cross-Reactivity, Specificity, and Binding Mechanisms" (featured on the cover) *Journal of Molecular Biology* **414**, 385-400 (2011).

53. N. M. Levinson, E. E. Bolte, C. S. Miller, S. A. Corcelli, and S. G. Boxer, "Phosphate Vibrations Probe Local Electric Fields and Hydration in Biomolecules," (communication) *Journal of the American Chemical Society* **133**, 13236 (2011).

54. M. Sajadi, K. E. Furse, X.-X. Zhang, L. Dehmel, S. A. Kovalenko, S. A. Corcelli, and N. P. Ernsting, "Detection of DNA-Ligand Binding Oscillations by Stokes-Shift Measurements" (communication) *Angewandte Chemie International Edition* **50**, 9501 (2011).

55. R. A. Nicodemus, S. A. Corcelli, J. L. Skinner, and A. Tokmakoff, "Collective Hydrogen Bond Reorganization in Water Studied with Temperature-Dependent Ultrafast Infrared Spectroscopy," *Journal of Physical Chemistry B* **115**, 5604 (2011).

56. K. E. Furse and S. A. Corcelli, "Dynamical Signature of Abasic Damage in DNA," (communication) *Journal of the American Chemical Society* **133**, 720 (2011).

57. K. E. Furse and S. A. Corcelli, "Effects of an Unnatural Base Pair Replacement on the Structure and Dynamics of DNA and Neighboring Water and Ions," *Journal of Physical Chemistry B* **114**, 9934 (2010).

58. C. S. Miller and S. A. Corcelli, "Carbon-Deuterium Vibrational Probes of the Protonation State of Histidine in the Gas-Phase and in Aqueous Solution," *Journal of Physical Chemistry B* **114**, 8565 (2010).

59. K. E. Furse and S. A. Corcelli, "Molecular Dynamics Simulations of DNA Solvation Dynamics," (perspective featured on the cover) *Journal of Physical Chemistry Letters* **1**, 1813 (2010).

60. H. A. Fox, K. E. Newman, W. F. Schneider, and S. A. Corcelli, "Bulk and Surface Properties of Rutile TiO_2 from Self-Consistent-Charge Density Functional Tight Binding," *Journal of Chemical Theory and Computation* **6**, 499 (2010).

61. K. E. Furse and S. A. Corcelli, “Effects of Long-Ranged Electrostatics on Time-Dependent Stokes Shift Calculations,” *Journal of Chemical Theory and Computation* **5**, 1959 (2009).

62. B. A. Lindquist, K. E. Furse, and S. A. Corcelli, “Nitrile Groups As Vibrational Probes of Biomolecular Structure and Dynamics: An Overview,” (perspective featured on the cover) *Physical Chemistry Chemical Physics* **11**, 8119 (2009).

63. C. S. Miller and S. A. Corcelli, “Carbon-Deuterium Vibrational Probes of Amino Acid Protonation State,” (letter) *Journal of Physical Chemistry B* **113**, 8218 (2009).

64. C. S. Miller, E. A. Ploetz, M. E. Cremeens, and S. A. Corcelli, “Carbon-Deuterium Vibrational Probes of Peptide Conformation: Alanine Dipeptide and Glycine Dipeptide,” *Journal of Chemical Physics* **130**, 125103 (2009).

65. B. A. Lindquist, R. T. Haws, and S. A. Corcelli, “Optimized Quantum Mechanics/Molecular Mechanics Strategies for Nitrile Vibrational Probes: Acetonitrile and *para*-Tolunitrile in Water and Tetrahydrofuran,” *Journal of Physical Chemistry B* **112**, 13991 (2008).

66. K. E. Furse and S. A. Corcelli, “The Dynamics of Water at DNA Interfaces: Computational Studies of Hoechst 33258 Bound to DNA,” *Journal of the American Chemical Society* **130**, 13103 (2008).

67. B. A. Lindquist and S. A. Corcelli, “Nitrile Groups as Vibrational Probes: Calculations of the C≡N Infrared Absorption Line Shape of Acetonitrile in Water and Tetrahydrofuran,” (letter) *Journal of Physical Chemistry B* **112**, 6301 (2008).

68. J. R. Schmidt and S. A. Corcelli, “Infrared Absorption Line Shapes in the Classical Limit: A Comparison of the Classical Dipole and Fluctuating Frequency Approximations,” *Journal of Chemical Physics* **128**, 184504 (2008).

69. K. E. Furse, B. A. Lindquist, and S. A. Corcelli, “Solvation Dynamics of Hoechst 33258 in Water: An Equilibrium and Nonequilibrium Molecular Dynamics Study,” *Journal of Physical Chemistry B* **112**, 3231 (2008).

70. C. S. Kinnaman, M. E. Cremeens, F. E. Romesberg, and S. A. Corcelli, “Infrared Line Shape of an α-Carbon Deuterium-Labeled Amino Acid,” (communication) *Journal of the American Chemical Society* **128**, 13335 (2006).

71. S. Li, J. R. Schmidt, S. A. Corcelli, C. P. Lawrence, and J. L. Skinner, “Approaches for the Calculation of Vibrational Frequencies in Liquids: Comparisons to Benchmarks for Azide/Water Clusters,” *Journal of Chemical Physics* **124**, 204110 (2006).

72. S. A. Corcelli and J. L. Skinner, “Infrared and Raman Line Shapes of Dilute HOD in Liquid H_2O and D_2O from 10 to 90 °C,” *Journal of Physical Chemistry A* **109**, 6154 (2005).

73. J. R. Schmidt, S. A. Corcelli, and J. L. Skinner, “Pronounced Non-Condon Effects in the Ultrafast Infrared Spectroscopy of Water,” *Journal of Chemical Physics* **123**, 044513 (2005).

74. J. B. Asbury, T. Steinel, S. A. Corcelli, C. P. Lawrence, J. L. Skinner, and M. D. Fayer, "Dynamics of Water Probed with Vibrational Echo Correlation Spectroscopy" *Journal of Chemical Physics* **121**, 12431 (2004).

75. J. R. Schmidt, S. A. Corcelli, and J. L. Skinner, "Ultrafast Vibrational Spectroscopy of Water and Aqueous *N*-methylacetamide: Comparison of Different Electronic Structure/Molecular Dynamics Approaches" *Journal of Chemical Physics* **121**, 8887 (2004).

76. S. A. Corcelli, C. P. Lawrence, J. B. Asbury, T. Steinel, M. D. Fayer, and J. L. Skinner, "Spectral Diffusion in a Fluctuating Charge Model of Water" *Journal of Chemical Physics* **121**, 8897 (2004).

77. J. B. Asbury, T. Steinel, C. Stromberg, S. A. Corcelli, C. P. Lawrence, J. L. Skinner, and M. D. Fayer, "Water Dynamics: Vibrational Echo Correlation Spectroscopy and Comparison to Molecular Dynamics Simulations" (featured on the cover) *Journal of Physical Chemistry A* **108**, 1107 (2004).

78. T. Steinel, J. B. Asbury, S. A. Corcelli, C. P. Lawrence, J. L. Skinner, and M. D. Fayer, "Water Dynamics: Dependence on Local Structure Probed with Vibrational Echo Correlation Spectroscopy" *Chemical Physics Letters* **386**, 295 (2004).

79. S. A. Corcelli, C. P. Lawrence, and J. L. Skinner, "Combined Electronic Structure/Molecular Dynamics Approach for Ultrafast Infrared Spectroscopy of Dilute HOD in Liquid H_2O and D_2O" *Journal of Chemical Physics* **120**, 8107 (2004).

80. S. A. Corcelli, J. A. Rahman, and J. C. Tully, "Efficient Thermal Rate Constant Calculation for Rare Event Systems" *Journal of Chemical Physics* **118**, 1085 (2003).

81. S. A. Corcelli and J. C. Tully, "Vibrational Energy Pooling in CO on NaCl(100): Simulation and Isotope Effects" (featured on the cover) *Journal of Physical Chemistry A* **106**, 10948 (2002).

82. S. A. Corcelli, J. A. Kelley, J. C. Tully, and M. A. Johnson, "Infrared Characterization of the Icosahedral Shell Closing in $Cl^-\cdot H_2O\cdot Ar_n$ ($1 \leq n \leq 12$) Clusters" (featured on the cover) *Journal of Physical Chemistry A* **106**, 4872 (2002).

83. S. A. Corcelli and J. C. Tully, "Vibrational Energy Pooling in CO on NaCl(100): Methods and Simulation" *Journal of Chemical Physics* **116**, 8079 (2002).

84. L. R. Pratt, G. J. Tawa, G. Hummer, A. E. Garcia, and S. A. Corcelli, "Boundary Integral Methods for the Poisson Equation of Continuum Dielectric Solvation Models" *International Journal of Quantum Chemistry* **64**, 121 (1997).

85. S. A. Corcelli and J. D. Doll, "A Bayesian Approach to Short-Time Quantum Dynamics: Quantum Instantaneous Normal Modes" *Chemical Physics Letters* **263**, 671 (1996).

Peer-Reviewed Conference Proceedings (3 total)

1. C. S. Lent, K. W. Henderson, S. A. Kandel, S. A. Corcelli, G. L. Snider, A. O. Orlov, P. M. Kogge, M. T. Niemier, R. C. Brown, J. A. Christie, N. A. Wasio. R. C. Quardokus, R. P. Forrest, J. P. Peterson, A. Silski, D. A. Turner, E. P. Blair, and Y. Lu, "Molecular Cellular Networks: A Non von Neumann Architecture for

Molecular Electronics" *IEEE International Conference on Rebooting Computing (ICRC)*. San Diego: IEEE, 2016. 1-7.

2. J. D. Doll, M. Eleftheriou, S. A. Corcelli, and D. L. Freeman, "Equilibrium and Dynamical Path Integral Methods" *NATO Advances Study Institute on Quantum Monte Carlo Methods in Physics and Chemistry*. Dordrecht: Springer, 1999. 213-245.

3. S. A. Corcelli, J. D. Kress, L. R. Pratt, and G. J. Tawa, "Mixed Direct-Iterative Methods for Boundary Integral Formulations of Continuum Dielectric Solvation Models" *Biocomputing: Proceedings of the 1996 Pacific Symposium.* Singapore: World Scientific, 1996. 142-159.

Invited Presentations (96 total)

1. University of Illinois-Chicago, Chicago, Illinois, March 31, 2022: "Why is CO_2 Selectively Absorbed into Ionic Liquids?"

2. ACS Graduate Student and Postdoctoral Scholars Advisory Board (GSPSAB), American Chemical Society National Meeting, San Diego, California, March 21, 2022: "Abusive Mentoring in Graduate Training"

3. Notre Dame Learning | Kaneb Center for Teaching Excellence, University of Notre Dame, Notre Dame, Indiana, March 16, 2022: "How to Improve your Course Instructor Feedback (CIF) Scores"

4. 2022 Depression on College Campuses Conference (DoCC), Eisenberg Family Depression Center, University of Michigan, March 9-10, 2022: "Systemic Changes to Better Support Graduate Student Mental Health and Well-Being"

5. Telluride Workshop on Chemistry and Dynamics in Complex Environments, Telluride, Colorado, June 22-25, 2021: "Coupled Local Mode Approach for the Calculation of Vibrational Spectra: Application to Protonated Water Clusters"

6. American Chemical Society National Meeting, San Diego, California, August 25-29, 2019: "Why is CO_2 Selectively Absorbed into Ionic Liquids?"

7. European Center for Calculations on Atoms and Molecules (CECAM) workshop on Dynamics of Water in Complex Environments, Bridging the Gap Between Molecular and Mesoscopic Interfaces, École Normale Supérieure, Paris, France, July 15-17, 2019: "Computing the Infrared Spectra of Gas-Phase Protonated Water Clusters"

8. Telluride Workshop on Chemistry and Dynamics in Complex Environments, Telluride, Colorado, June 25-28, 2019: "Computing the Infrared Spectra of Gas-Phase Protonated Water Clusters"

9. Wintergreen Meeting of Physical Chemists, Wintergreen, Virginia, June 8-12, 2019: "Role of Counterions on Aqueous Hydroxide Mobility"

10. American Chemical Society National Meeting, Orlando, Florida, March 31-April 4, 2019: "Computational Vibrational Spectroscopy of Aqueous Acid and Base Solutions"

11. University of California-Berkeley, Berkeley, California, February 12, 2019: “Computational Vibrational Spectroscopy of Aqueous Acid and Base Solutions”

12. Pacific Conference on Spectroscopy and Dynamics, San Diego, California, January 24-27, 2019: “Computational Vibrational Spectroscopy of Aqueous Acid and Base Solutions”

13. Telluride Workshop on Advances of Multidimensional Vibrational Spectroscopy in Water, Biology and Materials Science, Telluride, Colorado, July 9-13, 2018: “Dynamics and Vibrational Spectroscopy of Molecular Reporters in Ionic Liquids”

14. Tufts University, Medford, Massachusetts, April 10, 2018: “Dynamics and Vibrational Spectroscopy of Molecular Reporters in Ionic Liquids”

15. American Chemical Society National Meeting, New Orleans, Louisiana, March 18-22, 2018: “Role of Quadrupolar Interactions in the Solvation of Carbon Dioxide in Ionic Liquids”

16. Rutgers University, New Brunswick, New Jersey, February 20, 2018: “Dynamics and Vibrational Spectroscopy of Molecular Reporters in Ionic Liquids”

17. Ohio State University, Columbus, Ohio, January 12, 2018: “Dynamics and Vibrational Spectroscopy of Molecular Reporters in Ionic Liquids”

18. Ohio State University, Columbus, Ohio, January 11, 2018: “Theoretical Approaches to Vibrational Spectroscopy in the Condensed Phase”

19. Ohio State University, Columbus, Ohio, January 10, 2018: “DNA and Phosphate Hydration”

20. Wichita State University, Wichita, Kansas, November 29, 2017: “Dynamics and Vibrational Spectroscopy of Molecular Reporters in Ionic Liquids”

21. Brown University, Providence, Rhode Island, November 16, 2017: “Dynamics and Vibrational Spectroscopy of Molecular Reporters in Ionic Liquids”

22. Femto13, Cancún, Mexico, August 12-17, 2017: “DNA Hydration: A Perspective from MD Simulations of Solvation Dynamics and Vibrational Spectroscopy”

23. Telluride Workshop on Chemistry and Dynamics in Complex Environments, Telluride, Colorado, June 26-29, 2017: “IR and Raman Spectroscopy of the Excess Proton in Aqueous Solution”

24. American Chemical Society National Meeting, San Francisco, California, April 2-6, 2017: “Dynamics and Vibrational Spectroscopy of Molecular Reporters in Ionic Liquids”

25. Western Michigan University, Kalamazoo, Michigan, November 7, 2016: “Ionic Liquid Dynamics”

26. University of Notre Dame (Department of Chemistry and Biochemistry Colloquium), Notre Dame, Indiana, September 29, 2016: “Ionic Liquid Dynamics”

27. Penn Conference on Theoretical Chemistry, Philadelphia, Pennsylvania, August 19-20, 2016: "Nonadiabatic Electron Transfer in Mixed-Valence Molecules"

28. Gordon Research Conference on Water and Aqueous Solutions, Holderness School, Holderness, New Hampshire, July 31 – August 5, 2016: "DNA Hydration: A Perspective from MD Simulations of Solvation Dynamics and Vibrational Spectroscopy"

29. 2nd Joint Notre Dame-Heidelberg Summer School in Computational Chemistry, Notre Dame, Indiana, July 4-9, 2016: "Molecular Dynamics Simulations of Biomolecules"

30. École Normale Supérieure, Paris, France, April 28, 2016: "DNA Hydration: A Perspective from MD Simulations of Solvation Dynamics and Vibrational Spectroscopy"

31. Purdue University, West Lafayette, Indiana, October 7, 2015: "Dynamics and Vibrational Spectroscopy of Water, Alcohols, and Carbon Dioxide in Ionic Liquids"

32. University of Notre Dame (Condensed Matter Physics Seminar), Notre Dame, Indiana, October 1, 2015: "Simulations of Rare Events in Nonadiabatic Systems"

33. American Chemical Society National Meeting, Boston, Massachusetts, August 16-20, 2015: "Dynamics and Spectroscopy of Water, Alcohols, and Carbon Dioxide in Ionic Liquids"

34. Telluride Workshop on Chemistry and Dynamics in Complex Environments, Telluride, Colorado, June 23-26, 2015: "Simulations of Rare Events in Nonadiabatic Systems"

35. University of Pittsburgh, Pittsburgh, Pennsylvania, October 9, 2014: "Solvation Dynamics and Vibrational Spectroscopy in Ionic Liquids"

36. University of Rochester, Rochester, New York, September 22, 2014: "Solvation Dynamics and Vibrational Spectroscopy in Ionic Liquids"

37. American Chemical Society National Meeting, San Francisco, California, August 10-14, 2014: "Solvation Dynamics and Vibrational Spectroscopy in Ionic Liquids"

38. Telluride Workshop on Interfacial Molecular and Electronic Structure and Dynamics, Telluride, Colorado, July 7-11, 2014: "DNA Hydration: A Perspective from MD Simulations of Solvation Dynamics"

39. Dynamics and Spectroscopy in the Condensed Phase: Celebrating Jim Skinner's 60th Birthday symposium, University of Wisconsin, Madison, Wisconsin, May 20-21, 2014: "Molecular Dynamics Investigation of the Vibrational Spectroscopy of Isolated Water in an Ionic Liquid"

40. Pacific Conference on Spectroscopy and Dynamics, Asilomar Conference Center, Pacific Grove, California, January 30 - February 2, 2014: "DNA Hydration: A Perspective from MD Simulations of Solvation Dynamics"

41. Telluride Workshop on Chemistry and Dynamics in Complex Environments, Telluride, Colorado, June 25-29, 2013: "Solvation Dynamics in Ionic Liquids"

42. Midwest Theoretical Chemistry Conference, University of Illinois at Urbana-Champaign, May 30, 2013: "Solvation Dynamics in Ionic Liquids"

43. Michigan State University, East Lansing, Michigan, October 9, 2012: "Solvation Dynamics in Ionic Liquids"

44. Telluride Workshop on Interfacial Molecular and Electronic Structure and Dynamics, Telluride, Colorado, July 2-6, 2012: "Solvation Dynamics in Ionic Liquids"

45. American Chemical Society National Meeting, San Diego, California, March 25-29, 2012: "Toward Transition Path Sampling with Surface Hopping"

46. Sustainable Energy Initiative Seminar, University of Notre Dame, Notre Dame, Indiana, September 26, 2011: "Solvation Dynamics in Ionic Liquids"

47. American Conference on Theoretical Chemistry, Telluride, Colorado, July 18-22, 2011: "Solvation Dynamics in DNA"

48. Telluride Workshop on Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, Colorado, July 4-8, 2011: "Dynamical Signature of Abasic Damage in DNA"

49. Telluride Workshop on Chemistry and Dynamics in Complex Environments, Telluride, Colorado, June 26-30, 2011: "Dynamical Signature of Abasic Damage in DNA"

50. Central Regional Meeting of the American Chemical Society, Indianapolis, Indiana, June 8, 2011: "Computational Studies of Infrared Probes of Protonation State and Hydration"

51. European Center for Calculations on Atoms and Molecules (CECAM) workshop on Vibrational Spectroscopy of Complex Systems, École Normale Supérieure, Paris, France, May 23-25, 2011: "Computational Studies of Infrared Probes of Protonation State and Hydration"

52. University of California, San Diego, California, May 3, 2011: "Dynamical Signature of Abasic Damage in DNA"

53. Haverford College, Haverford, Pennsylvania, April 15, 2011: "Dynamical Signature of Abasic Damage in DNA"

54. 17th Annual German-American Kavli Frontiers of Science Symposium, Irvine, California, April 9-11, 2011: Poster: "Dynamics of DNA Hydration and Damage: A Computational Study of Coumarin 102/DNA"

55. Pacifichem 2010, Honolulu, Hawaii, December 15-20, 2010: "Dynamical Signature of Abasic Damage in DNA"

56. California Institute of Technology, Pasadena, California, December 7, 2010: "Dynamical Signature of Abasic Damage in DNA"

57. University of Southern California, Los Angeles, California, December 6, 2010: "Dynamical Signature of Abasic Damage in DNA"

58. Gonzaga University, Spokane, Washington, November 5, 2010: “Dynamical Signature of Abasic Damage in DNA”

59. Colorado State University, Fort Collins, Colorado, October 21, 2010: “Dynamical Signature of Abasic Damage in DNA”

60. University of Colorado, Boulder, Colorado, October 22, 2010: “Dynamical Signature of Abasic Damage in DNA”

61. University of Nevada, Reno, Nevada, October 19, 2010: “Dynamical Signature of Abasic Damage in DNA”

62. Northwestern University, Evanston, Illinois, October 6, 2010: “Dynamical Signature of Abasic Damage in DNA”

63. University of Texas, Austin, Texas, October 4, 2010: “Dynamical Signature of Abasic Damage in DNA”

64. University of Notre Dame (Department of Chemistry and Biochemistry Seminar), Notre Dame, Indiana, September 21, 2010: “Dynamical Signature of Abasic Damage in DNA”

65. Gordon Research Conference on Vibrational Spectroscopy: Probing Structure and Dynamics, University of New England, Biddeford, Maine, August 1-6, 2010: “Theoretical Studies of Vibrational Probes of Biomolecular Structure and Dynamics”

66. American Chemical Society National Meeting, San Francisco, California, March 22, 2010: “Dynamics of DNA Hydration and Damage: A Computational Study of Coumarin 102/DNA”

67. Greater Boston Area Theoretical Chemistry Lecture Series (co-sponsored by Boston University, Harvard University, and the Massachusetts Institute of Technology), Boston, Massachusetts, March 10, 2010: “Computational Spectroscopy of Biomolecular Hydration, Structure, and Dynamics”

68. University of Illinois, Urbana-Champaign, Illinois, March 3, 2010: “Computational Studies of DNA Hydration Dynamics”

69. University of Notre Dame (Condensed Matter Physics Seminar), Notre Dame, Indiana, February 18, 2010: “Computational Studies of DNA Hydration Dynamics”

70. Purdue University, West Lafayette, Indiana, February 10, 2010: “Computational Studies of DNA Hydration Dynamics”

71. Brown University, Providence, Rhode Island, November 12, 2009: “Computational Studies of DNA Hydration Dynamics”

72. University of Pennsylvania, Philadelphia, Pennsylvania, October 22, 2009: “Computational Studies of DNA Hydration Dynamics”

73. Franklin and Marshall College, Lancaster, Pennsylvania, October 21, 2009: “Vibrational Probes of Biomolecular Structure and Dynamics”

74. University of Rochester, Rochester, New York, October 19, 2009: “Computational Studies of DNA Hydration Dynamics”

75. University of Kansas, Lawrence, Kansas, October 9, 2009: “Vibrational Probes of Biomolecular Structure and Dynamics”

76. University of Missouri-Columbia, Columbia, Missouri, October 8, 2009: “Computational Studies of DNA Hydration Dynamics”

77. Georgia Tech, Atlanta, Georgia, September 29, 2009: “Vibrational Probes of Biomolecular Structure and Dynamics”

78. Emory University, Atlanta, Georgia, September 28, 2009: “Computational Studies of DNA Hydration Dynamics”

79. American Chemical Society National Meeting, Washington D.C., August 20, 2009: “Computational Studies of Hydration Dynamics at the DNA Interface: Hoechst 33258/DNA and Coumarin 102/DNA”

80. Telluride Workshop on Chemistry and Dynamics in Complex Environments, Telluride, Colorado, June 25, 2009: “Computational Studies of Hydration Dynamics at the DNA Interface: Hoechst 33258/DNA and Coumarin 102/DNA”

81. Great Lakes Regional Meeting of the American Chemical Society, Lincolnshire, Illinois, May 15, 2009: “Computational Studies of Hydration Dynamics at the DNA Interface: Hoechst 33258/DNA and Coumarin 102/DNA”

82. Proteins and Water Workshop, Arizona State University, Tempe, Arizona, May 13, 2009: “Computational Studies of Hydration Dynamics at the DNA Interface: Hoechst 33258/DNA and Coumarin 102/DNA”

83. University of Michigan, Ann Arbor, Michigan, November 10, 2008: “Computational Studies of Solvation Dynamics at DNA Interfaces”

84. Ohio State University, Columbus, Ohio, October 20, 2008: “Computational Studies of Solvation Dynamics at DNA Interfaces”

85. Grand Valley State University, Allendale, Michigan, September 12, 2008: “Computational Studies of Solvation Dynamics at DNA Interfaces”

86. Advances in Chemical Dynamics Workshop Honoring Jimmie D. Doll, Santa Fe, New Mexico, August 14, 2008: “Computational Studies of Solvation Dynamics at DNA Interfaces”

87. Central Regional Meeting of the American Chemical Society, Columbus, Ohio, June 13, 2008: “Computational Studies of Solvation Dynamics at DNA Interfaces”

88. American Chemical Society National Meeting, New Orleans, Louisiana, April 9, 2008: "Computational Studies of Solvation Dynamics at DNA Interfaces"

89. University of Notre Dame (Physical Chemistry Seminar), Notre Dame, Indiana, February 21, 2008: "Spectroscopic Probes of the Structure and Dynamics of Biomolecules"

90. University of Wisconsin, Madison, Wisconsin, October 1, 2007: "Spectroscopic Probes of the Structure and Dynamics of Biomolecules"

91. American Chemical Society National Meeting, Boston, Massachusetts, August 23, 2007: "Solvation Dynamics at DNA Interfaces"

92. Telluride Workshop on Vibrational Dynamics, Telluride, Colorado, August 6, 2007: "Computational Studies of C_α-D and C≡N Vibrational Probes"

93. Hillsdale College, Hillsdale, Michigan, April 4, 2006: "Computational Methods for the Vibrational Spectroscopy of Proteins"

94. Telluride Workshop on Vibrational Dynamics of Biological Molecules, Telluride, Colorado, August 14, 2005: "Computational Approaches to Vibrational Spectroscopy: Benchmark Calculations for Azide/Water"

95. Telluride Workshop on Ultrafast Nonlinear Spectroscopy in Fluids, Telluride, Colorado, June 26, 2005: "Non-Condon Effects in the Ultrafast Vibrational Spectroscopy of Water"

96. Gordon Research Conference on Computational Chemistry, Holderness School, Plymouth, New Hampshire, July 4, 2004: "Computational Strategies for Ultrafast Vibrational Spectroscopy: Applications to Water and Aqueous Solutions"

Contributed Presentations (14 total)

1. Biophysical Society Annual Meeting, San Francisco, California, February 19-23, 2022: "Elucidating the Binding Mechanism of Hoechst 33258 to a DNA Duplex"

2. American Chemical Society National Meeting, San Francisco, California, April 2-6, 2017: "Nonadiabatic Electron Transfer in Mixed-Valence Molecules"

3. American Physical Society National Meeting, New Orleans, March 13, 2017: "Phosphate Vibrations as Reporters of DNA Hydration"

4. Pacifichem 2015, Honolulu, Hawaii, December 20, 2015: "The Role of Protein Flexibility in Immunogenic Recognition"

5. American Chemical Society National Meeting, Indianapolis, Indiana, September 8, 2013: "Computational Investigation of Phosphate Vibrations as Reporters of the Onset of Hydration in DNA"

6. American Chemical Society National Meeting, San Diego, California, March 28, 2012: “Solvation Dynamics in Ionic Liquids”

7. American Chemical Society National Meeting, San Diego, California, March 26, 2012: “Computational Studies of Infrared Probes of Protonation State and Proton Transfer”

8. American Chemical Society National Meeting, Anaheim, California, March 30, 2011: “Dynamical Signature of Abasic DNA Damage: A Computational Study of Coumarin 102 in DNA”

9. American Chemical Society National Meeting, Anaheim, California, March 28, 2011: “Computational Studies of Infrared Probes of Amino Acid Protonation State”

10. Gordon Research Conference on Water and Aqueous Solutions, Holderness School, Holderness, New Hampshire, August 8, 2010: Poster: “Dynamics of DNA Hydration and Damage: A Computational Study of Coumarin 102/DNA”

11. American Chemical Society National Meeting, Philadelphia, Pennsylvania, August 21, 2008: “Computational Studies of Solvation Dynamics at DNA Interfaces”

12. American Chemical Society National Meeting, Chicago, Illinois, March 29, 2007: “Computational Studies of C_α-D Vibrational Probes in Peptides”

13. American Chemical Society National Meeting, San Francisco, California, September 10, 2006: “Infrared Line Shapes of C_α-D Labeled Amino Acids”

14. Gordon Research Conference on Vibrational Spectroscopy: Probing Structure and Dynamics, University of New England, Biddeford, Maine, July 2, 2006: Poster: “Infrared Line Shapes of Carbon-Deuterium (C-D) Labeled Amino Acids: Alanine in Aqueous Solution”

External Research Support

S. A. Corcelli (PI) and Paul S. Cremer (co-PI), “Collaborative Research: Ion Mobility in Aqueous Acids, Bases, and Salts,” National Science Foundation, 6/1/2022 – 5/31/2025, $720,000 ($375,000 to Notre Dame)

S. A. Corcelli (PI), “Dynamics and Vibrational Spectroscopy of Ionic Liquids Mixtures,” National Science Foundation, 9/1/16 – 8/31/20, $464,036

S. A. Corcelli (PI), “Counterion Effects in Acidic and Basic Solutions,” National Science Foundation XSEDE, 4/1/19 – 6/30/20, $13,672

B. M. Baker (PI), S. A. Corcelli, K. W. Henderson, M. S. Stack, and R. E. Taylor, “GAANN Fellowships to Increase Diversity and Promote Academic Careers in the University of Notre Dame Department of Chemistry and Biochemistry,” Department of Education, 8/16/13 – 8/15/17, $704,480

S. A. Corcelli (PI), “Solvation Dynamics in Ionic Liquids,” American Chemical Society – Petroleum Research Fund, 9/1/12 – 8/31/16, $100,000

S. A. Corcelli (PI), "Nonadiabatic Transition Path Sampling (NAPS)," Sloan Research Fellowship, 09/15/09 – 09/14/11, $50,000

S. A. Corcelli (PI), "CAREER: Computational Studies of Water Dynamics at DNA Interfaces," National Science Foundation, 2/1/09 – 1/31/15, $512,276

S. A. Corcelli (PI), "Biological Water at DNA Interfaces," Northwest Indiana Computational Grid, 9/1/08 – 8/31/09, $25,000

S. A. Corcelli (PI), "Computational Studies of Hydrogen-Bond Dynamics in Methanol and Ethanol Probed by Ultrafast Infrared Spectroscopy," American Chemical Society – Petroleum Research Fund, 7/1/08 – 6/30/10, $50,000

S. A. Corcelli (PI), "New Theoretical and Computational Methods for Studying Electron and Proton Transfer in Confined Environments," Camille and Henry Dreyfus New Faculty Award, 9/1/05 – 8/31/10, $50,000

Internal Research Support

W. F. Schneider (PI), E. J. Maginn (co-PI), J. D. Gezelter (co-PI), J. K. Whitmer (co-PI), S. A. Corcelli (co-PI), Y. J. Colón (co-PI), A. W. Dowling (co-PI), Y. Zhang (co-PI), and H. Ma (co-PI), "Renewal of High-Performance Compute Clusters of the Computational Molecular Science and Engineering Laboratory," University of Notre Dame Equipment Restoration and Renewal Program, 5/1/2022 – 4/30/2023, $202,525

S. A. Corcelli (PI) and E. J. Maginn (co-PI), "Rapid Calculation of Isotherms for Absorption of Gases into Reactive Ionic Liquids," University of Notre Dame Sustainable Energy Initiative, 7/1/14 – 6/30/16, $71,000

S. A. Corcelli (PI), "Molecular Dynamics Simulations of Solvation Dynamics in Ionic Liquids," University of Notre Dame Sustainable Energy Initiative, 5/16/11 – 5/14/13, $64,667

S. A. Corcelli (PI), K. E. Newman (co-PI), and W. F. Schneider (co-PI), "Towards Simulating Chemical and Photochemical Reactions for Clean Energy: Methodologies for the Solid-Aqueous Interface," University of Notre Dame Energy Center, 9/1/08 – 08/31/09, $40,000

Courses Instructed (28 total)

1. CHEM 60641: Statistical Mechanics I, Spring 2022
2. CHEM 60641: Statistical Mechanics I, Spring 2021
3. CHEM 10171: Introduction to Chemical Principles, Fall 2019
4. CHEM 10171: Introduction to Chemical Principles, Fall 2018
5. CHEM 60648: Quantum Mechanics II, Spring 2018
6. CHEM 60640: Math Methods for the Chemical and Life Sciences, Fall 2017
7. CHEM 20262: Mathematical Methods for the Chemical Sciences, Spring 2017
8. CHEM 60641: Statistical Mechanics I, Fall 2016
9. CHEM 14221: British Discoveries in Chemistry and Their Modern Impacts, University of Notre Dame London Undergraduate Program, Spring 2016
10. CHEM 60641: Statistical Mechanics I, Fall 2015
11. CHEM 60648: Quantum Mechanics II, Spring 2015

12. CHEM 30337: Physical Chemistry for the Life Sciences, Fall 2014
13. CHEM 60648: Quantum Mechanics II, Spring 2014
14. CHEM 30337: Physical Chemistry for the Life Sciences, Fall 2013
15. CHEM 60649: Quantum Mechanics I, Fall 2012
16. CHEM 60641: Statistical Mechanics I, Fall 2012
17. CHEM 60648: Quantum Mechanics II, Spring 2012
18. CHEM 60641: Statistical Mechanics I, Fall 2011
19. CHEM 30322: Physical Chemistry II, Spring 2011
20. CHEM 30321: Physical Chemistry I, Fall 2010
21. CHEM 20262: Mathematical Methods for the Chemical Sciences, Spring 2010
22. CHEM 60649: Quantum Mechanics I, Fall 2009
23. CHEM 60641: Statistical Mechanics I, Fall 2008
24. CHEM 20262: Mathematical Methods for the Chemical Sciences, Spring 2008
25. CHEM 60641: Statistical Mechanics I, Fall 2007
26. CHEM 60648: Quantum Mechanics II, Spring 2007
27. CHEM 60641: Statistical Mechanics I, Fall 2006
28. CHEM 60649: Quantum Mechanics I, Fall 2005

Mentoring

Postdoctoral Research Associates (3 total)

1. Kristina (Furse) Davis (2006-2010)
2. Hannah Fox (2008-2010)
3. Ryan Mullen, co-advised by Ed Maginn (2015-2018)

Graduate Students (21 total)

1. Cory Ayres, co-advised by Brian Baker (Ph.D. 2017)
2. Lindsay Baxter (M.Sc. 2015)
3. Shelby Brantley (Ph.D. 2020)
4. Erin (Groth) Brossard (2019-present)
5. Olivia Cracchiolo, co-advised by Arnaldo Serrano (Ph.D. 2021)
6. Clyde Daly (Ph.D. 2018)
7. Danyal Floisand (Ph.D. 2017)
8. Ryan Forrest (M.Sc. 2017)
9. Matthew Hanson (2018-present)
10. Ryan Haws (Ph.D. 2012)
11. Shanghui Huang (2017-2018)
12. Paul Johns (2007-2008)
13. Nell Karpinski (2022-present)
14. Laura Kinnaman, co-advised by Kathie Newman (Ph.D. 2011)
15. Carrie (Kinnaman) Miller (Ph.D. 2010)
16. Tierney Miller (Ph.D. 2020)
17. Ruth Nelson, co-advised by Brian Baker (M.Sc. 2016)
18. Jacob Petersen, co-advised by S. Alex Kandel (Ph.D. 2021)
19. Janel Reed (M.Sc. 2020)

20. Mary Sherman (Ph.D. 2015)
21. Zachary Terranova (Ph.D. 2014)
22. Jonathan Walker, co-advised by David Bartels (M.Sc. 2016)
23. Shuang Wu (2022-present)

Undergraduate Students (24 total)

1. Cecelia Allison, Notre Dame (2015-2018)
2. Erin Bolte, Notre Dame (2010-2012)
3. Bonnie Chow, Notre Dame (2008-2010)
4. Brian Conway, Notre Dame (2011-2012)
5. Ceren Germeyan, REU student from Bowdoin College (summer 2006)
6. Zachary Goldstein, REU student from Yeshiva University (summer 2011)
7. Scott Gustafson, REU student from UCSD, co-advised by Kathie Newman (summer 2007)
8. Frances Mei Hardin, Notre Dame (2010-2012)
9. Erik Helgesen, Notre Dame (2010-2011)
10. Emily Herman, Saint Mary's College (2007-2008)
11. Cameron Houk, Notre Dame (2011-2012)
12. Dana Hulke, Notre Dame (2010-2012)
13. Tesia Janicki, Notre Dame (2012-2016)
14. Daniel Kovacs, REU student from Pazmany Peter Catholic University, Hungary (summer 2007)
15. Beth Lindquist, Notre Dame (2006-2007)
16. Molly (Smith) Malloy, Notre Dame (2008-2010)
17. Jenna Morgan, Notre Dame (2017-2019)
18. Daniel Pardo, Notre Dame (2020-present)
19. Elizabeth Ploetz, REU student from Kansas State University (summer 2007)
20. Brittni Qualizza, Saint Mary's College (summer 2008)
21. Madison Sendzik, Saint Mary's College (summer 2018)
22. Alexis Stensby, Notre Dame (2019-2021)
23. Lauren (Schilling) Tuffy, Notre Dame (2008-2010)
24. Elbert Williams, Notre Dame (2008-2010)

Professional Service and Leadership

2022 – present	Telluride Science Research Center Board of Directors
2019	Condensed Phase and Interfacial Molecular (CPIMS) Program Review, Pacific Northwest National Laboratory, Department of Energy
2019	Co-organizer of the 51st Midwest Theoretical Chemistry Conference, University of Notre Dame, Notre Dame, Indiana, June 6-8, 2019
2018 – present	American Chemical Society Graduate Education Board
2017	Review Panel, Division of Chemistry, National Science Foundation
2017	Cottrell Scholars Collaborative Academic Leadership Training Workshop
2017	Organizer of the "Multicenter Molecules and Coupled Molecular Assemblies – Synthesis, Characterization, and Theory" symposium, American Chemical Society National Meeting, San Francisco, California, April 2-6, 2017
2016 – 2021	*The Journal of Physical Chemistry Letters* Editorial Advisory Board
2015 – 2017	Chair, American Chemical Society Graduate Education Advisory Board

2015 – 2018	*The Journal of Physical Chemistry* Editorial Advisory Board
2015	Editorial in the July 2015 *ACS Graduate and Postdoctoral Chemist*, "Why Every Graduate Student and Postdoctoral Scholar Needs an Individual Development Plan (IDP)"
2015	National Diversity Equity Workshop, Washington D.C.
2015	Awards Committee for the PHYS Division of the American Chemical Society
2015	Review Panel, Division of Chemistry, National Science Foundation
2015	Past-Chair, Biophysical Subdivision of the American Chemical Society
2014	Awards Committee for the PHYS Division of the American Chemical Society
2014	Vice-Chair, American Chemical Society Graduate Education Advisory Board
2014	Guest editor of the J. L. Skinner Festschrift for *The Journal of Physical Chemistry*
2014	Chair, Biophysical Subdivision of the American Chemical Society
2014	Co-organizer of the "Dynamics and Spectroscopy in the Condensed Phase: Celebrating Jim Skinner's 60th Birthday" symposium, University of Wisconsin, Madison, Wisconsin, May 20-21, 2014
2013	Chair-Elect, Biophysical Subdivision of the American Chemical Society
2012 – 2013	American Chemical Society Graduate Education Advisory Board
2012	Vice-Chair, Biophysical Subdivision of the American Chemical Society
2012	Co-organizer of the "Solvent Dynamics at Biomolecular Interfaces: Experiment and Theory" symposium, American Chemical Society National Meeting, Philadelphia, Pennsylvania, August 19-23, 2012
2011	Co-organizer of the 43rd Midwest Theoretical Chemistry Conference, University of Notre Dame, Notre Dame, Indiana, June 9-11, 2011
2011	Review Panel, Division of Chemistry, National Science Foundation
2008	Co-organizer of the "Spectroscopic Probes of Chemical Dynamics in Gaseous and Condensed Phase" symposium, American Chemical Society National Meeting, Philadelphia, Pennsylvania, August 17-21, 2008
2005 – present	Refereed proposals for the National Science Foundation, Department of Energy, Research Corporation, American Chemical Society Petroleum Research Fund, and the United States Civilian Research and Development Foundation
2005 – present	Refereed papers for *Science*, *Nature Communications*, *Nature Chemistry*, *Nature Chemical Biology*, *Journal of the American Chemical Society*, *Proceedings of the National Academy of Sciences U.S.A.*, *Accounts of Chemical Research*, *Chemical Reviews*, *Biophysical Journal, Biochemistry, Journal of Chemical Physics*, *Journal of Physical Chemistry*, *Journal of Physical Chemistry Letters*, *Journal of Chemical Theory and Computation*, *Langmuir, Structural Dynamics, International Reviews in Physical Chemistry*, *Chemical Physics*, *Chemical Physics Letters*, *PLoS ONE*, *Theoretical Chemistry Accounts*, *Chemical Society Reviews, ACS Books, Biopolymers,* and *Journal of Molecular Structure*
2005	Judge for the Midwest Regional Finals of the Siemens Westinghouse Competition in Math, Science, and Technology

University Service and Leadership

2022	Teaching, Professor of the Practice, Advisor, Clinical, Research, and Library Faculty Promotions Review Committee
2021 – 2022	Insider Threat Working Group, University of Notre Dame
2020 – 2021	Strategic plan working group, College of Science, University of Notre Dame

2020 – 2021	William K. Warren Foundation Dean of the College of Science Search Committee, University of Notre Dame
2020 – 2021	General Chemistry Teaching Faculty Search Committee, Department of Chemistry and Biochemistry, University of Notre Dame
2020 – 2021	Chair, Theoretical Chemistry Faculty Search Committee, Department of Chemistry and Biochemistry, University of Notre Dame
2020 – 2022	Faculty Fellow, Kaneb Center for Teaching Excellence, University of Notre Dame
2020 – 2021	COVID-19 response at the University of Notre Dame: Research and Graduate Studies Task Force Research Laboratory Operations Task Force Graduate Student Continuity Group Emotional Support and Wellbeing Working Group Student Funds and Employment Working Group
2019 – present	College Council, College of Science, University of Notre Dame
2019 – 2020	Chair, Task Force on Mentoring and Anti-Bullying, University of Notre Dame
2019 – 2020	Chair, Task Force on Graduate Student Well-Being, University of Notre Dame
2019 – present	Center for Research Computing Faculty Advisory Committee, University of Notre Dame
2019 – 2021	Fellow, Office of the Provost, University of Notre Dame
2019	Sister Kathleen Cannon Distinguished Lecture Series Selection Committee, University of Notre Dame
2019	Chair, Five-Year Dean of Science Review Committee, University of Notre Dame
2018 – 2021	University Committee on Women Faculty and Students, University of Notre Dame
2018	Naughton Fellowship Selection Committee, University of Notre Dame
2017 – 2019	Committee on Appointments and Promotions, Department of Chemistry and Biochemistry, University of Notre Dame
2016 – 2019	Chair, Strategic Planning Committee, Department of Chemistry and Biochemistry, University of Notre Dame
2016 – 2019	Associate Chair, Department of Chemistry and Biochemistry, University of Notre Dame
2015 – 2016	ND LEAD Program, University of Notre Dame
2014 – present	Space Committee, Department of Chemistry and Biochemistry, University of Notre Dame
2013 – 2017	Co-Administrator of the Department of Chemistry and Biochemistry Graduate Assistance in Areas of National Need (GAANN) program, University of Notre Dame
2012 – 2014	Vision Committee, Department of Chemistry and Biochemistry, University of Notre Dame
2012 – 2013	English for Academic Purposes Advisory Committee, University of Notre Dame
2012 – 2016	Director of Graduate Studies, Department of Chemistry and Biochemistry, University of Notre Dame
2011 – 2016	Integrated Biomedical Sciences Program Steering Committee, University of Notre Dame
2011 – 2013	College of Science Computing Committee, University of Notre Dame
2010 – 2011	University of Notre Dame Committee on Academic Technologies
2010 – 2011	Chair, College of Science Computing Committee, University of Notre Dame
2008 – 2010	Center for Research Computing Software Subcommittee, University of Notre Dame
2008 – 2011	Graduate Studies Committee, Department of Chemistry and Biochemistry, University of Notre Dame
2008 – 2010	Physical Chemistry Seminar Coordinator, Department of Chemistry and Biochemistry, University of Notre Dame
2007 – 2008	Center for Research Computing Faculty Advisory Committee, University of Notre Dame

2007	Faculty participant in the Physics REU program, University of Notre Dame
2006 – 2007	Faculty participant in the Nano Bioengineering REU program, University of Notre Dame
2005 – 2008	Graduate Recruitment Committee, Department of Chemistry and Biochemistry, University of Notre Dame